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Effect of the number of shells on the pressure and energy of two-dimensional free bubble clusters

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Abstract

We have performed Surface Evolver simulations of two-dimensional hexagonal bubble clusters consisting of a central bubble of area λ surrounded by s shells or layers of bubbles of unit area. Clusters of up to twenty layers have been simulated, with λ varying between 0.01 and 100. In monodisperse clusters (*i.e.*, for λ=1) [1] both the average pressure of the entire cluster and the pressure in the central bubble are decreasing functions of s and approach 0.9306 for very large s, which is the pressure in a bubble of an infinite monodisperse honeycomb foam. Here we address the effect of changing the central bubble area λ. For small λ the pressure in the central bubble and the average pressure were both found to decrease with s, as in monodisperse clusters. However, for large λ, the pressure in the central bubble and the average pressure increase with s. The average pressure of large clusters was found to be independent of λ and to approach 0.9306 asymptotically.
We have also determined the cluster surface energies given by the equation of equilibrium for the total energy in terms of the area and the pressure in each bubble. When the pressures in the bubbles are not available, an approximate equation derived by Vaz *et al*. [2] was shown to provide good estimations for the cluster energy provided the bubble area distribution is narrow. This approach does not take cluster topology into account. Using this approximate equation, we find a good correlation between Surface Evolver simulations and the estimated values of energies and pressures.

Keywords: Clusters, Surface Evolver, bubbles, foams

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1. Introduction

Two-dimensional bubble clusters, either periodic or with a free boundary, have attracted attention in recent years [1-5], particularly in relation to the effect of the size and arrangement (*i.e.* topology) of the bubbles on the energy (perimeter) and stability of the clusters. Free monodisperse clusters consisting of N bubbles of equal area were studied [3] in an attempt to find the topology of lowest energy (the so-called minimal perimeter problem) and the optimal shape of the periphery of an otherwise hexagonal cluster. Small periodic and free bidisperse and polydisperse clusters were also studied with the aim of finding energetic groundstates [2, 4, 5].

The total cluster perimeter, or energy E_c, of a two-dimensional cluster is given by the equilibrium equation [6]

$$E_c = 2\sum_i A_i p_i \qquad (1)$$

as a function of the area A_i and the pressure p_i in each bubble. In an earlier paper [1], theoretical estimates and Surface Evolver simulation results were presented for the energies and the bubble pressures of monodisperse hexagonal foam clusters. These consist of a central bubble surrounded by s shells of bubbles, each bubble having unit area. The total number of bubbles in such a cluster is $N=3s^2+3s+1$. Upper and lower bounds for the average pressure were also derived, and these agreed with Surface Evolver calculations [1]. It was found that, as N becomes large, the average bubble pressure approaches a limiting value. This value was derived in earlier work [1], but can be briefly explained. In an infinite regular honeycomb lattice consisting of identical bubbles of edge length L and area A, we have $A/L^2=3^{3/2}/2$. As shown by Hales [7], the minimum perimeter enclosing N bubbles of unit area is $3NL$. The energy per bubble in an infinite honeycomb is thus $2^{1/2}3^{1/4} \approx 1.8612$, hence the energy per bubble in a very large but finite honeycomb cluster will approach 1.8612. If we apply the equation of equilibrium in 2D (Eq. 1), with $A=1$, we obtain that the average pressure is $2^{-1/2}3^{1/4}\approx 0.9306$ [1].

The natural question to address next is how these conclusions change when the cluster is no longer monodisperse. Here we consider the simplest case of bidispersity, while retaining a high degree of cluster symmetry: we change the area A_c of the central bubble, while keeping

all others areas fixed at A=1 without loss of generality. The ratio $\lambda=A_c/A$ is varied between 0.01 and 100 for clusters of up to 20 shells.

We restrict our work to unstrained clusters. If we were to strain the foam, e.g., by removing bubbles and stretching the foam to close the resulting gap, the energies and the pressures would be affected in a non-trivial way.

The results for the variation of cluster energy and bubble pressure λ are presented in section 2, and we discuss the implications in section 3.

2. Results

We used the Surface Evolver program [8] to study the clusters. Examples of Surface Evolver-generated clusters with λ=10 and s shells are given in Fig. 1. For each λ, we start from an ordered cluster with the correct bubble areas and converge to a minimum of energy, allowing topological changes to occur when edges shrink to zero length.

The clusters have a six-fold axis of symmetry and a (free) boundary along close-packed rows of the hexagonal lattice. Fig. 2 shows two clusters with s=20 and two different central bubble areas, respectively λ=0.1 and λ=100. In this range of λ, they retain their full six-fold rotational symmetry, although all bubbles are not equivalent: in particular, peripheral bubbles have fewer than six neighbours; those located at the corners of the cluster have fewer still. For very high values of λ, clusters may undergo other topological arrangements with different symmetries from the six-fold ones. Such symmetries will not be discussed here.

We started by checking our numerical results against Eq. (1). The relative differences between the calculated energies E_c and the Surface Evolver energies E_e are less than 10^{-7}. Since Eq. (1) is exact, this provides a stringent test of the accuracy of our numerical results.

Fortes *et al.* [1] reported, on the basis of Surface Evolver calculations, that the pressure in the central bubble of a monodisperse hexagonal cluster decreases with the number of shells s and attains for infinite s the limiting value 0.9306. Fig. 3a shows the pressure in the central bubble p_0, vs the number of shells s, for several λ. For $\lambda\leq 10$, p_0 decreases with increasing s, as in the monodisperse cluster; for $\lambda>10$, however, p_0 becomes an increasing function of s. The same is true of the average pressure $\overline{p}$ over the entire s-shell cluster, see Fig. 3b.

Remarkably, the average pressure in a 20-shell cluster is almost independent of λ, even for large central bubble areas. It seems safe to conclude that in a large cluster the average pressure does not depend on λ and tends to the same limiting value, 0.9306, as in the monodisperse cluster [1]. To our knowledge this had not been seen before, and we regard it as a key result of this work. By contrast, the pressure in the central bubble p_0 does depend on λ for $\lambda>10$.

The value of λ at which the central bubble's pressure begins to increase with s, and is no longer independent of λ, appears to be correlated with the onset of topological changes. That is, when λ becomes large, there must be local changes in topology to accommodate the large central bubble, and the cluster is no-longer ordered. The induced disorder, although small, is probably more representative of real foams, and therefore the behaviour at large λ may be more typical. The dynamics of the process of changing λ [9] gives information about the sequences of topological changes that occur, and in particular whether the same paths through the energy landscape are repeated during cycles of inflation and deflation.

Vaz *et al.* [2] proposed an approximate equation for the surface energy of a bubble cluster:

$$E = \frac{3.722}{2}\sum_i A_i^{1/2} + 2.042\left(\sum_i A_i\right)^{1/2}. \qquad (2)$$

In this approach, the energy of the cluster is given in terms of the bubble areas A_i only, and does not depend on the cluster topology. Eq. (2) was found to be accurate for clusters with narrow area and edge length distributions; clusters with broader bubble area and edge length distributions are not well described [2]. To check whether this result applies to our hexagonal clusters, we plot $E/(\sum_i A_i)^{1/2}$ vs $\sum_i A_i^{1/2}/(\sum_i A_i)^{1/2}$ in Fig. 4. The straight line corresponds to the predictions of Eq. (2), while the dots represent the energies obtained with the Surface Evolver. It is clear that Eq. (2) provides a good account of our results, even for clusters with a large number of shells and large λ. This is perhaps not so surprising, as such clusters are actually "quasi-monodisperse": only one bubble – the central bubble – has different area and significantly different perimeter to the others, and as s or N increases this is a vanishingly small fraction of the total number of bubbles in the cluster.

Finally, we can estimate the average pressure in the cluster as

$$\bar{P}_{est} = \frac{E}{2\bar{A}N} \qquad (3)$$

where $\bar{A}$ is the average bubble area and E can be computed from Eq. (2). The differences between the average pressures given by the Surface Evolver, $\bar{P}_{sim}$, and the estimated average pressures, $\bar{P}_{est}$, from Eq. (3), are very small, see Fig. 5.

3. Conclusions

We have performed Surface Evolver simulations of two-dimensional hexagonal bubble clusters consisting of a central bubble of area λ surrounded by s shells or layers of bubbles of unit area. Results were found to be in excellent agreement with the equilibrium equation for the total cluster energy. Unlike in a monodisperse cluster, the pressure in the central bubble is no longer a monotonically decreasing function of the number of shells in the cluster for all λ. In fact, if λ is larger than a limiting value, the pressure in the central bubble increases with the number of shells. For clusters with a large number of shells, the average pressure in the cluster was found to tend to a common asymptotic value, namely the pressure in a monodisperse infinite honeycomb foam. An approximate equation for the surface energy of weakly polydisperse clusters has been shown to provide a good fit to our data.

An analogy between our work and impurities/inclusions in grains in metallic materials can be made. For a given value of λ >1, the contribution of the impurity, for example to the average pressure, will be larger in a cluster with few shells compared with a more typical cluster with many shells. The same happens with inclusions in grains of small area, for which the presence of inclusions will substantially affect the material's properties. In order to have a better approach to metallic grains, it would be interesting to study confined clusters and to extend this analysis to three-dimensions.

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Figure Captions

Fig. 1- Monodisperse clusters: a central bubble with area λ = 10 surrounded by s shells of unit-area bubbles: (a) s=1, (b) s=2, (c) s=3, (d) s=4, (e) s=7, (f) s=10, (g) s=15 and (h) s=20.

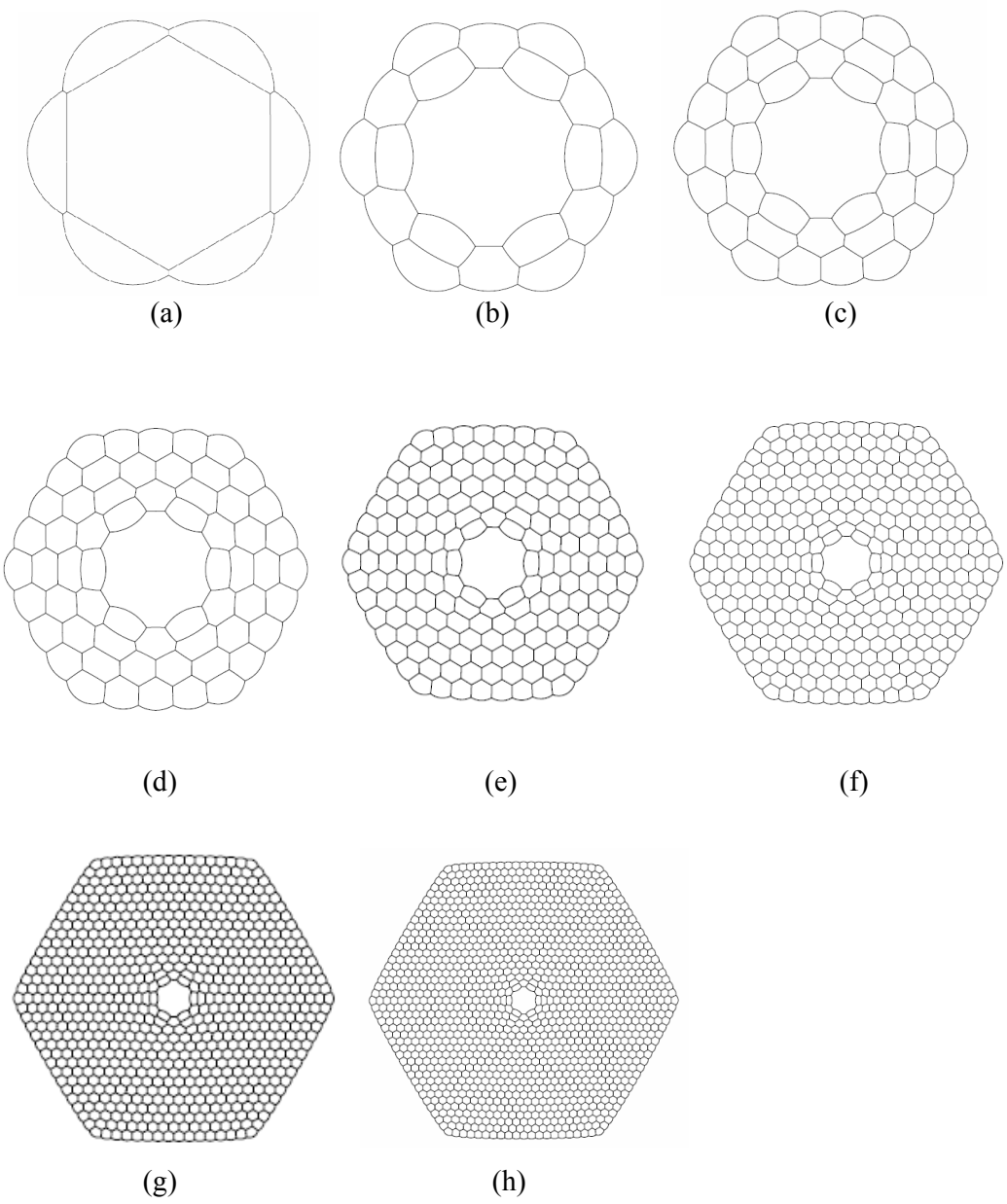
Fig. 2 - Clusters with N=1261 bubbles (s=20): (a) λ =0.1 and (b) λ = 100.

Fig. 3 - Pressures *vs* number of shells, s, for λ=0.01, 0.1, 0.5, 1, 3, 10, 15, 30, 50 and 100. (a) Pressure in the central bubble; (b) average pressure in the cluster.

Fig. 4 - $E/(\sum_i A_i)^{1/2}$ vs $\sum_i A_i^{1/2}/(\sum_i A_i)^{1/2}$. —— Energy given by Eq. (2), ♦ Energy given by the Surface Evolver simulations.

Fig. 5 - $(\bar{p}_{sim} - \bar{p}_{est})/N\lambda$ vs $\sum_i A_i^{1/2}/(\sum_i A_i)^{1/2}$. The differences between the pressures obtained in the simulations and the estimates of Eq. (3) are very small.

Figure(s)



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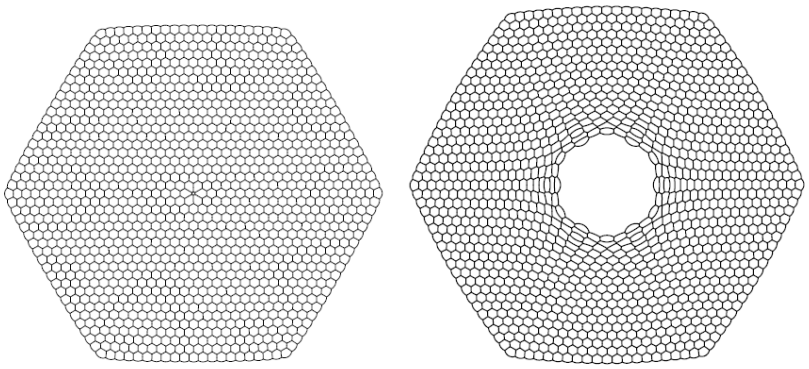
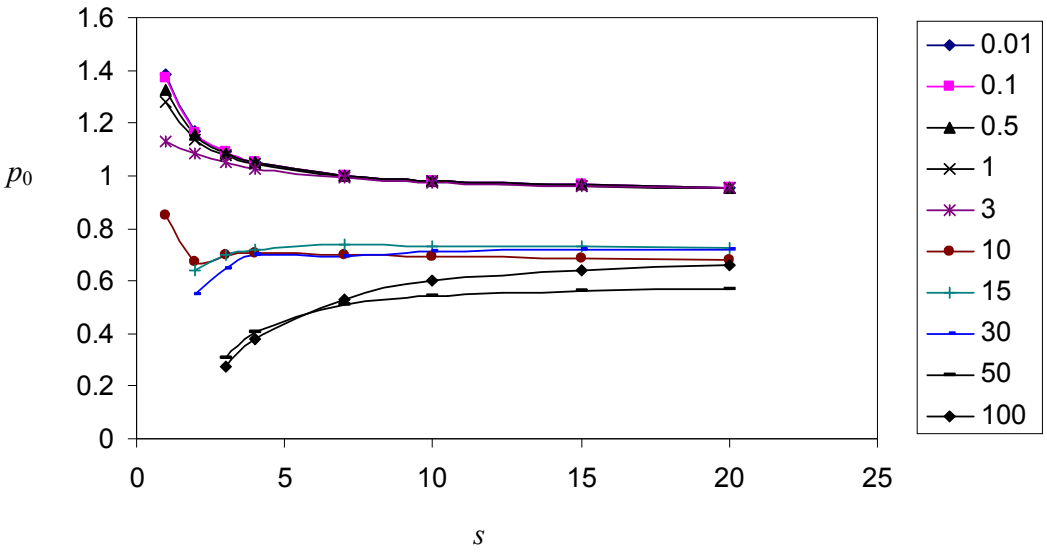
Figure(s)



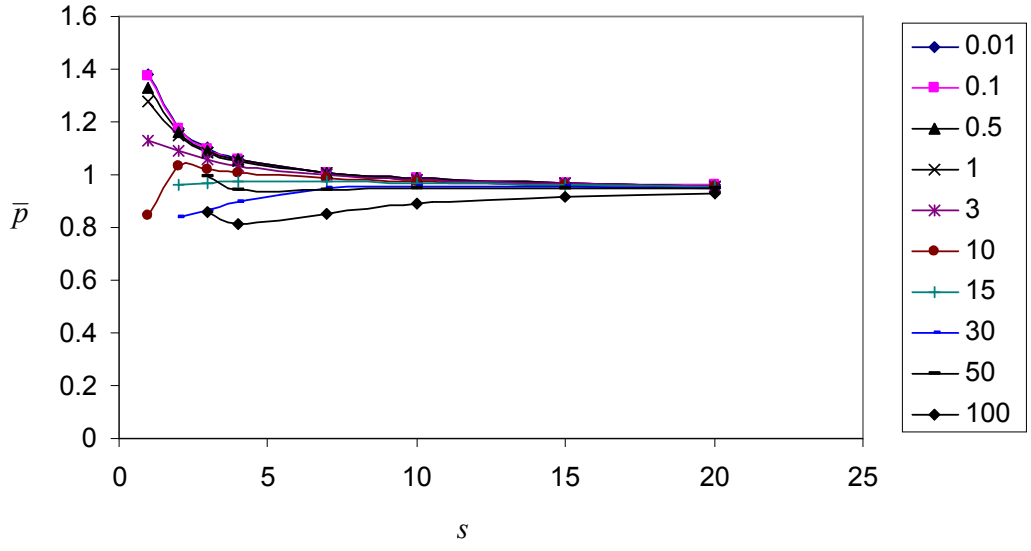
(a) (b)

Fig. 2 - Clusters with N=1261 bubbles (s=20): (a) λ =0.1 and (b) λ = 100.

Figure(s)



(a)



(b)

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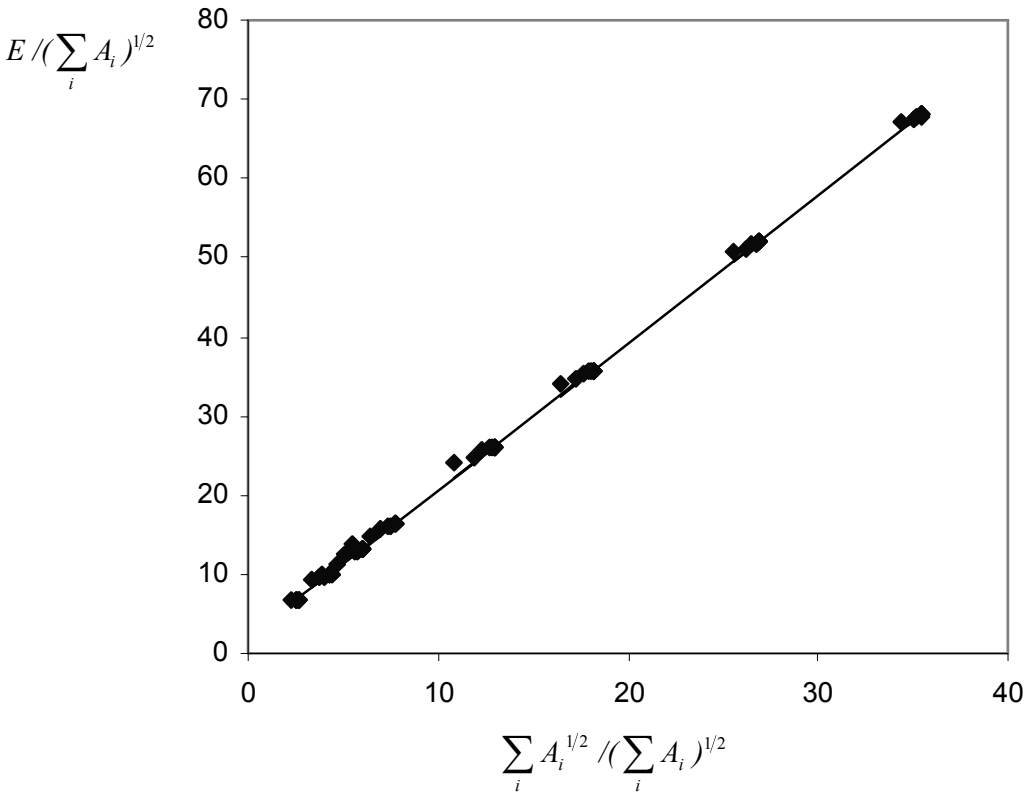

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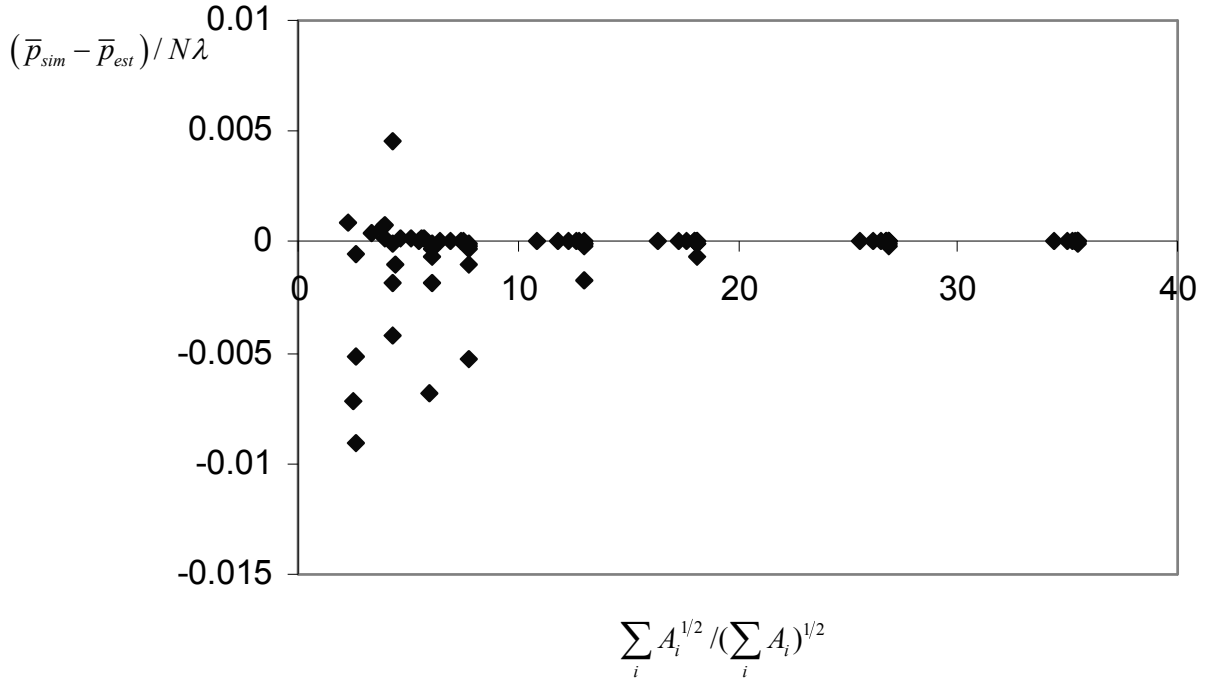

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